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Radiation Transport in 3D Heterogeneous Materials: Direct Numerical Simulation

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INTRODUCTION

The transport of particles (photons, neutrons, charged particles, neutrinos, etc) in a random medium is a very challenging problem that arises in a wide variety of applications. Astrophysics, atmospheric physics, biology and fusion science are just a few of the fields where this problem arises. Over the last 20 years, a theoretical framework has developed due in part to Levermore, Pomraning , Sanzo, Wong [1], Vanderhaegen [2], and others [3]. Even though the theoretical work has come along way in 20 years, it is still lacking in several important aspects. The models are exact only for transport with no scattering and for a chord length distribution which is Poisson. Unfortunately, for a lot of applications, neither of these criteria are met. Transport in a random medium for most cases is a 3D transport problem in a medium which does not have a chord length distribution which is Poisson. In turbulent flows for example, the chord length distribution tends to be Levy like [4], not Poisson. In addition, for many applications in fusion science and astrophysics, the medium is participating. This means there is an emission function which is a function of a material temperature which itself is coupled to the radiation field. Effectively, the coupling of matter to radiation looks like an effective scatterer. Admittedly, the theoretical models have been extended to include systems with scattering, however, these models still tend to be an approximation.

In order to understand the limitations of the theoretical models better and hopefully gain some insight into the problem of transport in a random medium, the goal of the work presented here is to develop a phenomenological picture based on direct numerical simulation. We present two examples of random media. One is computer generated based on an extension of the random walk algorithm. The other is based on hydrodynamic simulations of Rayleigh-Taylor unstable fluids. Only the former will be presented here. Using the radiography code HADES [4], we compute the attenuation of 10,000 incident rays upon a 100X100X100 mesh containing a statistical realization of the random medium. At the back plane of the mesh, the attenuation information is digitized and binned. We collect both the distribution of chord lengths through the material as well as the optical depth distribution. This process is repeated many times (~500). Each time a given statistical realization of the random medium is generated and a chord length and optical distribution are computed. These are then ensemble averaged to give an ensemble averaged optical depth distribution from which we compute an effective mean free path through the material.

Large multi-physics codes cannot typically afford to go off and solve a coupled transport problem along the lines of Levermore, Pomraning, and others. Typically, if a zone consists of two or more materials, they are assumed to be atomically mixed and the individual mean free paths are averaged using their respective volume fractions in order to form an average mean free path. This of course works well when the length scale for a typical material in a zone is small compared to the photon or neutron mean free path. However, as is well known, when the length scale of the inhomogeneity becomes comparable to the particle mean free path, the atomically averaged mean free path is an underestimation of the true mean free path. How are we then to include the effects of inhomogeneity in our codes? The ultimate goal of this work is to generate a table or series of multipliers on the atomically averaged opacity. Given some assumed or computed knowledge of the statistical nature of the medium, our goal is to generate a series of tables of opacity multipliers from the direct numerical simulation. In this paper we give a proof of principle of how this process would proceed.

1. GENERATING THE RANDOM MEDIUM: THE WORM CODE

The first step in performing transport through a heterogeneous medium is to consider how to generate the medium itself. Since our philosophy is to develop a semi-phenomenological approach to the transport problem it is highly desirable to have an algorithm with a few adjustable parameters that allows for some control of the statistical nature of the medium.. The algorithm we have chosen builds upon the random walk on a lattice in 3D and is designed to generate isotropic and anisotropic binary random media.. The user selects a volume fraction Vf, a mean length lambda, an assumed distribution F, and a radius R. The algorithm is illustrated schematically in Figure 1. We begin with a 3D cube of a single material A. The code (WORM) selects a statistically distributed length based on F and lambda. The next step is to randomly pick a zone and then populate all zones within a radius R with material B. If the length defined as the volume of material B raised to the 1/3 power does not exceed the statistically generated length scale, a direction is selected and the neighboring cells are populated with material B. The direction may be selected at random or with biasing. This process is repeated until the length scale has been met. The process is repeated until the volume fraction criterion is satisfied.

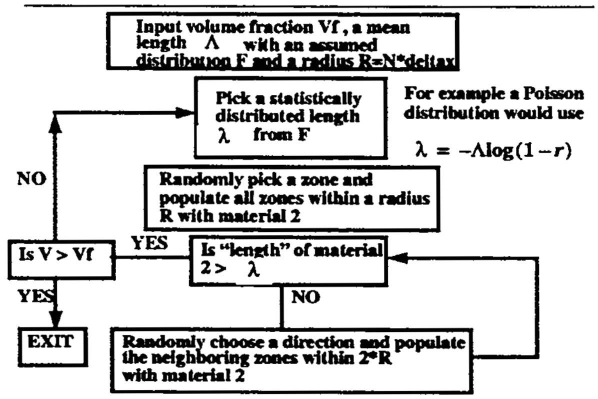

Figure 1.Flow chart diagram for the WORM code.

A wide variety of morphology can be generated with this method as is illustrated in Figure 2. These media represent a solid piece of iron with different types of void or cracks.

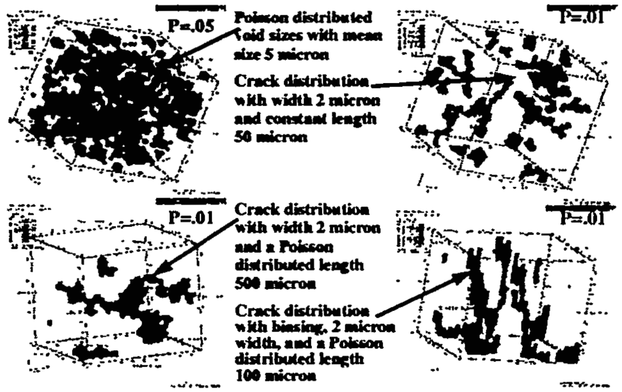

Fig. 2 Examples of random media generated with the algorithm described in Figure 1 and the text. P stands for porosity.

II. OPTICAL DEPTH DISTRIBUTION AND TRANSPORT THROUGH A RANDOM MATERIAL

With the random media generated, we use the radiography code HADES to compute attenuation through the material. The X-Rays chosen vary in energy from 4 keV to 1MeV. The rays enter on a given face of the cube. The examples shown above all consist of 100X100X100 zones. Hence a face presents 10,000 zones. HADES chooses one ray to enter each facial zone. Information concerning the attenuation is then collected at the far end of the cube. Of particular interest is the chord length distribution and the optical depth distribution. The former yields the statistical nature of the medium as experienced by a given ray. The latter yields the effective mean free path. Figure 3 shows an illustration of the type of process we go through to collect the required information.

The effective mean free path is computed from the optical depth distribution by realizing that

$$e^{-L/\lambda_{eff}} = \langle e^{-\tau} \rangle = \int d\tau F(\tau) e^{-\tau}$$

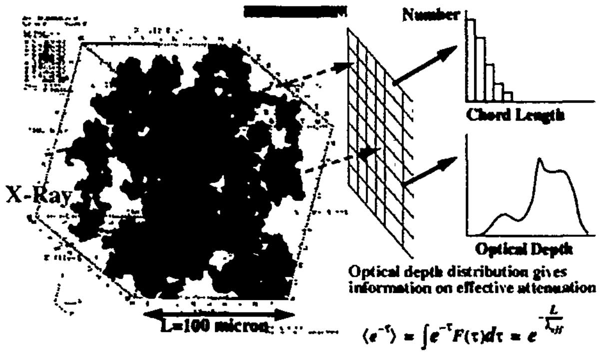

Fig.3 High energy x-rays are transported through the medium whereupon, the attenuation information is digitized. Chord length and optical depth distribution are computed.

In the example shown in Figure 4, an iron cube 100 micron by 100 micron by 100 micron is populated with a series of cracks. The volume fraction of cracks is 20%, the crack length is 1mm, and the photon energy is 4 keV. The statistical distribution of lengths is chosen in one case to be Poisson, in the other case it is Cauchy. In the former case, the ray sees a Poisson distribution of chord lengths. In the latter, the ray sees a chord length distribution that is Poisson with a power law behavior at large crack lengths. The optical depth distribution shows two optical depth distributions each centered about the homogenized or atomic value (dotted red line). The atomic value is the average optical depth taken from the optical depths of the two materials each weighted by their respective volume fractions. It is clear that as the optical depth distribution tends to a delta function, the effective mean free path attains the atomic value. The Cauchy distribution shows a wider distribution of optical depths. This is indicative of the fact that with Cauchy distributed random lengths, on average there will be more large length cracks when compared to Poisson. The wider tails of the distribution will tend to lower the effective mean free path.

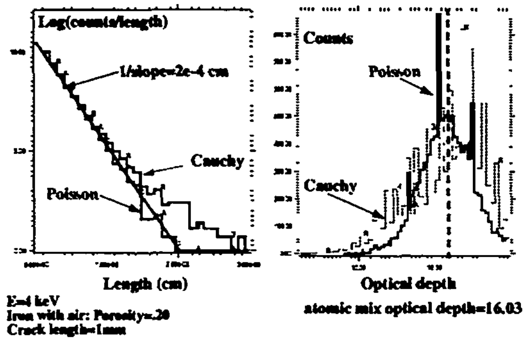

Fig. 4 Chord length and optical depth distribution for a 100 micron cube with cracks.

When the above process is repeated many times (>100) we generate a statistical ensemble of random media. It is from this statistical ensemble that we extract an average mean free path. In Figure 5, we show the optical depth distributions for Poisson and Cauchy distributed random media and the respective mean free paths. As expected, the shortest mean free path is exhibited by the atomic value of 6.24 microns. The Poisson distribution yields a mean free path of 6.94 micron and Cauchy distribution yields 7.05 microns.

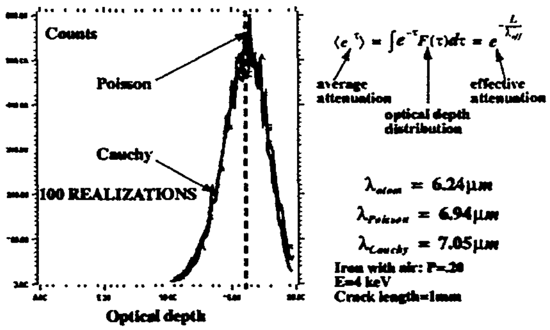

Fig. 5 Optical depth distribution and mean free paths for one hundred realizations

CONCLUSION

In order to develop a phenomenological approach to transport in 3D heterogeneous media, we have performed direct numerical simulation studies. Using an algorithm based on the lattice random walk to generate random media, we have performed radiographic shots of the sample and digitized both the chord length and optical depth distributions. The optical depth distribution is then used to compute an effective mean free path. As theory predicts, the atomically averaged mean free path is always a minimum value. We have also demonstrated a dependency of mean free path on the distribution of random material.

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